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Computational and experimental studies on strain induced effects in InGaAs/GaAs HFET structure using C–V profiling

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Abstract. We analyze strain induced effects on the capacitance-voltage (C–V) profile for MBE grown GaAs/$In_{0.1}Ga_{0.9}As$/GaAs HFET structure. The calculations of C–V profile were made using a small-signal approach developed for the quantum well (QW) structures. The self-consistent numerical simulations and results of measurements show that strain causes significant changes in the electron distribution of the QW structure and its C–V profile.

1. Introduction

Capacitance-voltage (C–V) profiling is on of the methods for the investigation and design of heterostructures quantum-well (QW) electronic and optoelectronic devices [1–5]. This technique is used for determining band offsets at the heterointerface. In the case of the psedomorphic structures, in particular, the GaAs/$In_{0.1}Ga_{0.9}As$/GaAs system, with sufficiently thin central layer the lattice constant mismatch is accommodated by internal strains rather than by formation of misfit dislocations. The strains lead to two consequences: the shifts of the conduction and valence bands in the well for the structures grown in [100] direction [6] and the built-in piezoelectric field for the structures grown in [111] direction [7]. However, with the exception of the Ref. [2], the calculations of band offsets from C–V experimental data were made without the strain effect. At the same time, the strain is sufficient large and produces the important changes in interband optical transitions [6]. The purpose of this work is to study the strain effect in GaAs/$In_{0.1}Ga_{0.9}As$/GaAs quantum-well HFET structure using the self-consistent numerical simulations and to compare the theoretical results with the measured C–V profile. The new simulation technique of the C–V characteristics for QW structures based on the small-signal approach [8] is developed.

2. Experiment

Experimental sample was grown by molecular beam epitaxy using a Riber32P system. Undoped GaAs layer with thickness 0.5 mm was used as a buffer. The conductive channel consists of n-GaAs (10 nm) followed by n-InGaAs (25 nm) and n-GaAs (75 nm) layers. Structure was capped by n-GaAs contact layer. The channel composition was optimized to obtain high linearity of the static and dynamic HFET characteristics. The process sequence for device fabrication is listed bellow:

1. Source and drain AuGa/Ni/Au contacts formation;
2. Device isolation by mesa etching and following proton implantation;
3. Gate electrode formation (E-beam lithography, gate recess and Ti/Pt/Au metallization);
4. Device passivation and contact pads metallization.

C–V profile for Schottky diode test structures (100 mm in diameter) was obtained from capacitance-voltage measurements at 1 MHz.

3. Theoretical model

The C–V (or apparent) profile N_{ap} (W) is given as usual by:

$$N_{ap} = -\frac{C^3(V)}{e\varepsilon(dC/dV)}, W(V) = \frac{\varepsilon}{C(V)}, \tag{1}$$

where e is the electron charge, ε is the semiconductor permittivity, and V is the reverse bias voltage applied to the Schottky barrier. Capacitance $C(V)$ can be calculated as [8]:

$$C(V) = \frac{\varepsilon}{W(V)} = \varepsilon\left(\frac{\int_0^L z\Delta n(z, V)dz}{\int_0^L \Delta n(z, V)dz}\right)^{-1} = \varepsilon\left(\int_0^L z\rho(z, V)dz\right)^{-1}, \tag{2}$$

where z is the space coordinate, L is the total structure thickness, and $\Delta n(z, V)$ is the perturbation of electron concentration due to the small voltage variation ΔV, ρ is the distribution function for the perturbed space charge density. Usually the perturbation $\Delta n(z, V)$ is calculated as the difference beetwen two static states $n(z, V + \Delta V)$ and $n(z, V)$ [3, 4]. Such approach demands the high accuracy and, consequently, the considerable computer resources. Recently we reported about very effective simulation technique of the barrier capacitance for the classical structures based on the small-signal approximation [8]. Now we applied this technique to the QW structure. In this case the electron concentration distribution $n(z, V)$ must be determined as the sum of the 3D and 2D concentrations, this later is obtained by following expression:

$$n_{2D}(z, V) = \sum_{i=1}^{m} |\Psi_i(z, V)|^2 n_i(V), \tag{3}$$

where m is number of bound states in QW, n_i is the electron occupation of state with eigenenergy E_i and wavefunction Ψ_i. The static 2D electron distribution is determined from the Schrödinger's equation. The Hamiltonian H in the effective-mass approximation for the conduction band can be written as [2]:

$$H = -\frac{\hbar^2}{2a(z)}\frac{d}{dz}\frac{a^2(z)}{m(z)}\frac{d}{dz}\frac{1}{a(z)} + V_{ef}(z), \tag{4}$$

were $a(z)$ and $m(z)$ are the position-dependent lattice constant and effective mass. The effective potential energy V_{ef} includes four terms:

$$V_{ef}(z) = E_c(z) + 2a_c\left(1 - \frac{C_{12}}{C_{11}}\right)\varepsilon_{xx} + eU(z) + V_{xc}(z), \tag{5}$$

were $E_c(z)$ is the conduction-band-edge energy, a_c is the hydrostatic deformation potential, C_{11} and C_{12} are the elastic stiffness constants, $\varepsilon_{xx} = \varepsilon_{yy}$ is the strain in the plane of the epitaxial growth [001], $V_{xc}(z)$ is the exchange-correlation energy. The Hartree electrostatic potential $U(z)$ is determined using the one-dimensional Boltzmann–Poisson equation. So, the calculation of the static electron distribution includes the quantum effects. After this, the barrier capacitance and apparent profile are simulated in the classical small-signal approximation [8]. The comparison of such "semi-classical" technique with the usual quasistatic approach gives that capacitance error is bellow 0.2%.

4. Results and discussion

In Fig.1 are presented the simulated 3D and 3D+2D electron distributions at the reverse bias $V = 0$ V. One cane see that the quantum effect changes the electron profile in the QW of HFET.

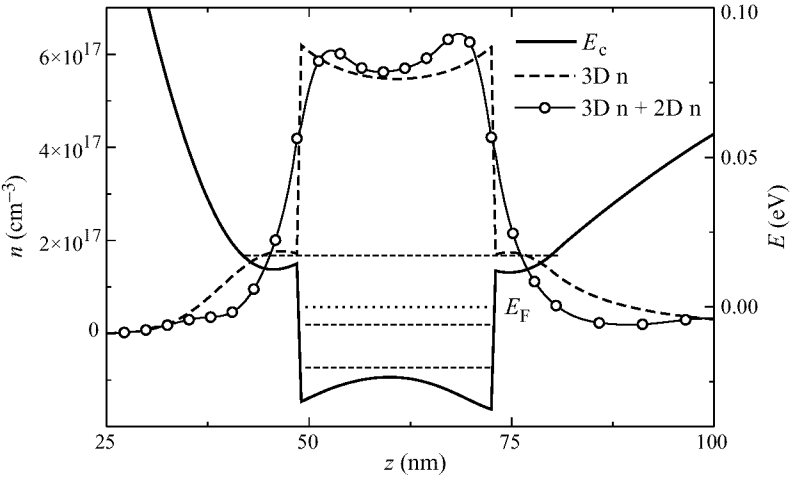

Fig. 1. Conduction-band-edge energy, lowest three sub-bands and electron distributions in QW.

Next Fig. 2 shows the results of C–V profiling and simulated apparent profiles for three cases: (i) unstrained QW; (ii) strained QW, the static electron distributions are calculated in classical approach; (iii) strained QW, the self-consistent simulation of the static electron distributions. On can conclude that strain effect makes the considerable influence to the apparent profile by the shift of conduction-band-edge energy in the QW. At the same time, the inclusion of the size effects produces the lesser influence for the given structure. The some discrepancy between the right slope of the simulated apparent profile and the experimental data cane be explicated by the effects of the edge capacitance and increasing

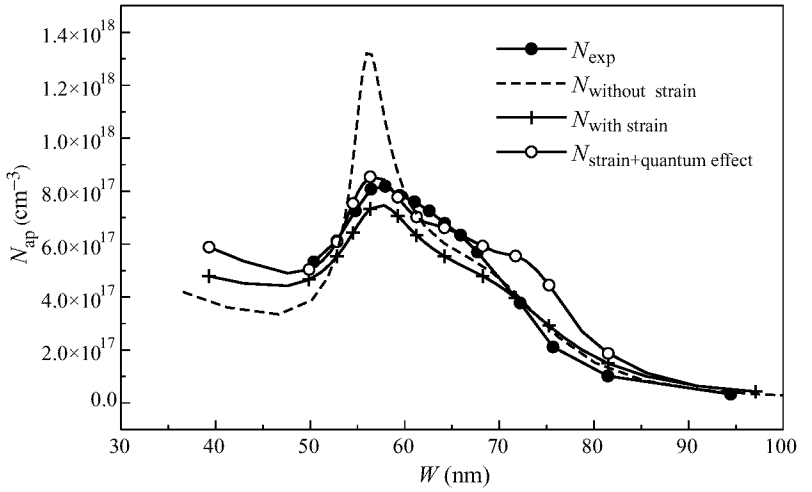

Fig. 2. Experimental and simulated apparent profiles.

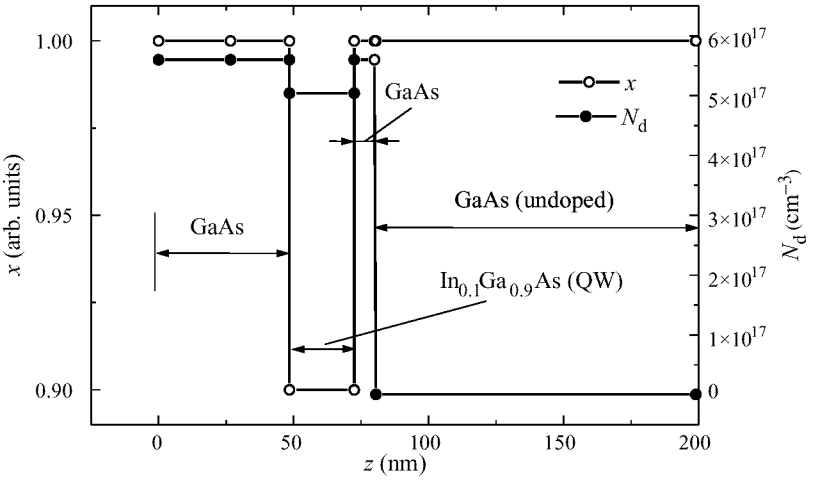

Fig. 3. Extracted mole fraction and doping profiles.

of the channel resistance. The extracted mole fraction and doping profiles are presented in Fig. 3.

The obtained thicknesses of the first GaAs n-layer is 48.5 nm and the second n-layer is 9 nm, the thickness of the QW is 24 nm. The doping level of the GaAs n-layers is $5.6 \cdot 10^{17}\,\mathrm{cm}^{-3}$. This results demonstrate the validity of the proposed "semi-classical" small-signal technique for the C–V profiling simulation of the real QW structures including strain effects.

Acknowledgments

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